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Nuclear Matrix Elements for Double- β Decay

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Recent progress in nuclear-structure theory has been dramatic. I describe recent and future applications of ab initio calculations and the generator coordinate method to double-beta decay. I also briefly discuss the old and vexing problem of the renormalization of the weak nuclear axial-vector coupling constant “in medium” and plans to resolve it.

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Neutrinoless double-beta ($0\nu\beta\beta$) decay occurs if neutrinos are Majorana particles, at a rate that depends on a weighted average of neutrino masses (see Refs. [1, 2] for reviews). New experiments to search for $0\nu\beta\beta$ decay are planned or underway. Extracting a mass from the results, however, or setting a reliable upper limit, will require accurate values of the nuclear matrix elements governing the decay. These cannot be measured and so must be calculated.

The matrix elements have been computed in venerable and sophisticated models, but vary by factors of two or three. All the models can be improved, however. Here I focus on two of them: the shell model and the generator coordinate method (GCM). I first discuss effective interactions and decay operators for the shell model that will connect that method to ab initio nuclear-structure calculations, which have made rapid progress recently. I then show how the GCM avoids problems of the quasiparticle random phase approximation (QRPA) and, moreover, can be extended so that it incorporates the QRPA's ability to capture proton-neutron pairing. Finally, I briefly examine the currently unsettling “renormalization” of the nuclear weak axial coupling constant g_A , and argue that the cause will be identified soon through and investigation of many-body currents and the effective enlargement of model spaces.

The lifetime for $0\nu\beta\beta$ decay, if the exchange of the familiar light neutrinos is responsible, is given by the product of a phase space factor (recently recomputed in Ref. [3]) an effective mass $m_\nu = \sum_i U_{ei}^2 m_i$, where m_i is the mass of the i^{th} eigenstate and U_{ei} weights each mass by the mixing angle of the associated eigenstate with the electron neutrino, and $M^{0\nu}$ is the nuclear matrix element. The matrix element is complicated but can be simplified without significantly altering its value through the “closure approximation.” In this approximation, and neglecting two-body currents (which I take up briefly later), one can write the matrix element as

$$M^{0\nu} = \frac{2R}{\pi g_A^2} \int_0^\infty q dq \quad (1)$$

$$\times \langle f | \sum_{a,b} \frac{j_0(qr_{ab}) [h_F(q) + h_{GT}(q) \vec{\sigma}_a \cdot \vec{\sigma}_b] + 3j_2(qr_{ab}) h_T(q) \vec{\sigma}_a \cdot \vec{r}_{ab} \vec{\sigma}_b \cdot \vec{r}_{ab}}{q + \bar{E} - (E_i + E_f)/2} \tau_a^+ \tau_b^+ | i \rangle ,$$

where $r_{ab} \equiv |\vec{r}_a - \vec{r}_b|$ is the distance between nucleons a and b , j_0 and j_2 are the usual spherical Bessel functions, \bar{E} is an average excitation energy to which the matrix element is insensitive, and the nuclear radius $R \equiv 1.2A^{1/3}$ fm is inserted with a compensating factor in the phase-space function to make the matrix element dimensionless. The “form factors” h_F , h_{GT} , and h_T are given in Refs. [4] and [5].

As already indicated, researchers have applied a variety of nuclear models to $\beta\beta$ decay. At the moment, it is difficult to assess the uncertainty in any one of the matrix-element calculations. Quantifying uncertainty is an important task for the next few years, but just as important is reducing the uncertainty by improving the calculations. We can do both by linking model Hamiltonians and decay operators

to data through ab initio calculations. The lighter $\beta\beta$ nuclei (^{76}Ge , ^{82}Se), or those such as ^{136}Xe that are near closed shells, will be the easiest to connect to ab initio work. The heavier nuclei will generally require a different treatment. I discuss those suitable for an ab initio treatment first.

The shell model is a complete diagonalization in a subspace of the full many-body Hilbert space that consists of all possible configurations of valence particles within a few valence single-particle orbitals, outside a core that is forced to remain inert. The model thus neglects excitations of the particles in the core into the valence levels or higher-lying levels, as well as excitations of the valence nucleons into higher-lying levels. At present, practitioners usually deal with this problem by constructing a phenomenological Hamiltonian for use in the shell model space. Nuclear-structure theory is reaching the point where we can do better, however. A variety of many-body methods now yield accurate solutions to the Schrödinger equation for nuclei with closed shells and nuclei with one or two nucleons outside closed shells. Among the methods are the coupled clusters approach [6] and the in-medium similarity renormalization group (IMSRG) [7]. These approaches can be used to construct, for up to two or three nucleons in the valence shell, a unitary transformation that transforms the full many-body Hamiltonian into block diagonal form, with a piece H_{eff} in the shell-model space that reproduces the lowest-lying energies exactly.

The procedure for obtaining the $0\nu\beta\beta$ matrix element in ^{76}Ge via a coupled-clusters-based shell-model calculation would go something like this:

1. Derive a two- and three-nucleon Hamiltonian from chiral effective field theory [8] or phenomenology in few-nucleon systems.
2. Do ab initio coupled-clusters calculations of the ground state of the closed shell nucleus ^{56}Ni , of the low-lying eigenstates of the closed-shell-plus-one nuclei ^{57}Ni and ^{57}Cu , and of the low-lying states of the closed-shell-plus-two nuclei ^{58}Ni , ^{58}Cu , and ^{58}Zn . Eventually, when it becomes possible, do the same in closed-shell+three nuclei as well.
3. Perform a “Lee-Suzuki” mapping [10] of the low-lying states in these nuclei onto states in the valence shell containing one and two (and eventually, three) nucleons. The mapping is designed to maximize the overlap of the full ab initio eigenstates with their shell-model images, while preserving orthogonality of the images [11].
4. Use the mapping of states to construct the shell-model interaction H_{eff} that gives the image states the same energies as their parents. Construct an effective double-beta operator that gives the same matrix elements between image states as the bare operator does between the associated parents.

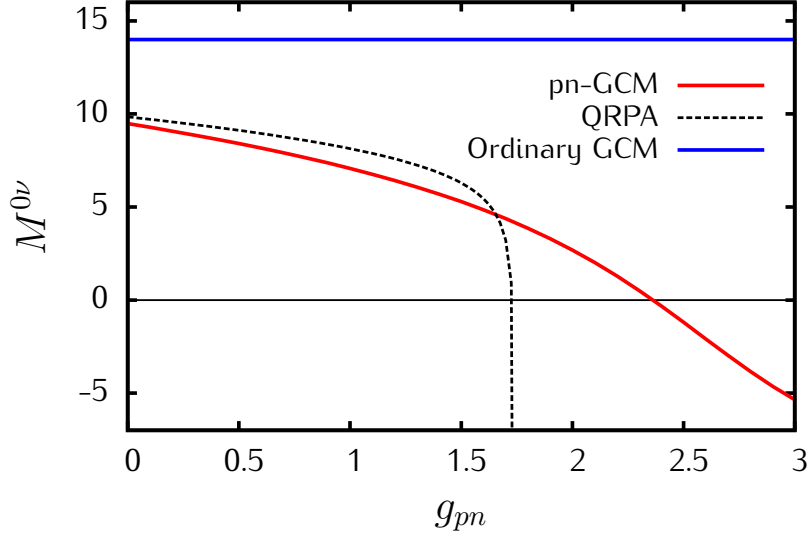


Figure 2: $0\nu\beta\beta$ matrix element for decay of ^{76}Ge in three models: the pn-QRPA (black dashed curve), the ordinary GCM without explicit proton-neutron correlations (flat blue solid line), and the GCM with proton-neutron pairing correlations (solid red curve). The quantity g_{pn} is the strength of the proton-neutron pairing in the Hamiltonian in Eq. (2). The quadrupole interaction in that Hamiltonian is turned off for this illustration. The calculations use two full oscillator shells as the single-particle model space.

two- and three-nucleon systems produces results which are at least as good. Though we have yet to investigate matrix elements of the double-beta operator, these initial results for energy levels are extremely promising. Including an effective three-nucleon interaction, from still extremely difficult ab initio calculations in ^{19}O and ^{17}C (ensuring that our predictions exactly match the ab initio results in those isotopes) should improve the spectra further. A larger shell model space would do the same. A similar program is being undertaken within the IMSRG [13].

For heavier complicated nuclei such as ^{130}Te or ^{150}Nd , fully ab initio calculations in the region are still a ways off. In those, we may have to use a more restricted wave function. Fortunately, recent work suggest that collective correlations may be most of what you need for an accurate matrix element [14]. The phenomenological methods, e.g., density functional theory, are built for collective correlations.

Such methods, particularly the GCM, have already been applied to $\beta\beta$ decay [15, 16], but not all collective correlations have been included. Neutron-proton pairing, in particular, is omitted because its effects are hard to see in nuclear spectra and transitions. It does, however, play a significant role in $\beta\beta$ decay. To see this, we have carried out calculation of the decay of ^{76}Ge in a Hilbert space consisting of 36

nucleons in two full oscillator shells with a semi-realistic interaction of the form

$$H = h_0 - \sum_{\mu=-1}^1 g_{\mu}^{T=1} S_{\mu}^{\dagger} S_{\mu} - \frac{\chi}{2} \sum_{K=-2}^2 Q_{2K}^{\dagger} Q_{2K} - g_{pn} \sum_{\nu=-1}^1 P_{\nu}^{\dagger} P_{\nu} + g_{ph} \sum_{\mu, \nu=-1}^1 F_{\nu}^{\mu\dagger} F_{\nu}^{\mu}, \quad (2)$$

where h_0 contains single particle energies, the Q_{2K} are components of the quadrupole operator, and

$$S_{\mu}^{\dagger} = \frac{1}{\sqrt{2}} \sum_l \sqrt{2l+1} [c_l^{\dagger} c_l^{\dagger}]_{00\mu}^{001}, \quad P_{\mu}^{\dagger} = \frac{1}{\sqrt{2}} \sum_l \sqrt{2l+1} [c_l^{\dagger} c_l^{\dagger}]_{0\mu 0}^{010}, \quad F_{\nu}^{\mu} = \frac{1}{2} \sum_i \sigma^{\mu}(i) \tau^{\nu}(i). \quad (3)$$

In this last line c_l^{\dagger} is a creation operator, l labels single-particle multiplets with good orbital angular momentum, S_{μ}^{\dagger} creates a correlated pair with total orbital angular momentum $L = 0$, spin $S = 0$, and isospin $T = 1$ (with μ labeling the isospin component $\tau = T_z$), P_{μ}^{\dagger} creates an isoscalar proton-neutron pair with $L = 0$ and $S = 1$ ($S_z = \mu$), and the F_{ν}^{μ} are the components of the Gamow-Teller operator. The Hamiltonian incorporates like-particle and proton-neutron pairing, a quadrupole-quadrupole interaction, and a repulsive “spin-isospin” interaction. Ref. [14] shows that in the fp shell, anyway, this kind of interaction reproduces full shell-model results accurately.

Fig. 2 shows the GCM results for the decay of ^{76}Ge ; the quadrupole interaction is temporarily turned off. The dashed curve is from the QRPA; it blows up when the proton-neutron pairing strength is near 1.5 (a realistic value). The reason is that the mean field on which the QRPA is based undergoes a phase transition from a condensate of like-particle pairs to a condensate of proton-neutron pairs at that point. The QRPA is unable to accommodate more than one mean field; it breaks down at the transition point. The GCM on the other hand, is explicitly designed to mix many mean fields. The technique is usually applied to nuclei that don’t have a definite shape (many $\beta\beta$ -decay candidates are in this class), with wave functions that are superpositions of states with a range of deformation. The GCM generates mean fields with that range by minimizing the mean-field energy under the constraint that the quadrupole moment take a particular value, then repeating the minimization for lots of other values for the quadrupole moment. The interaction is then diagonalized in the space of constrained mean-fields, usually after each has been projected onto states with well defined angular momentum and particle number.

The method as just described was applied together with the phenomenological density-dependent Gogny interaction to $0\nu\beta\beta$ decay in Refs. [15, 16]. The resulting matrix elements are usually larger than those of the shell model or QRPA. One reason is the absence of the proton-neutron correlations that in the QRPA shrink the matrix element as in Fig. 2 (before ruining it completely for very strong proton-neutron pairing). But one can add the physics of proton-neutron pairing by mixing together mean-fields (quasiparticle vacua) with different degrees of that pairing. One does

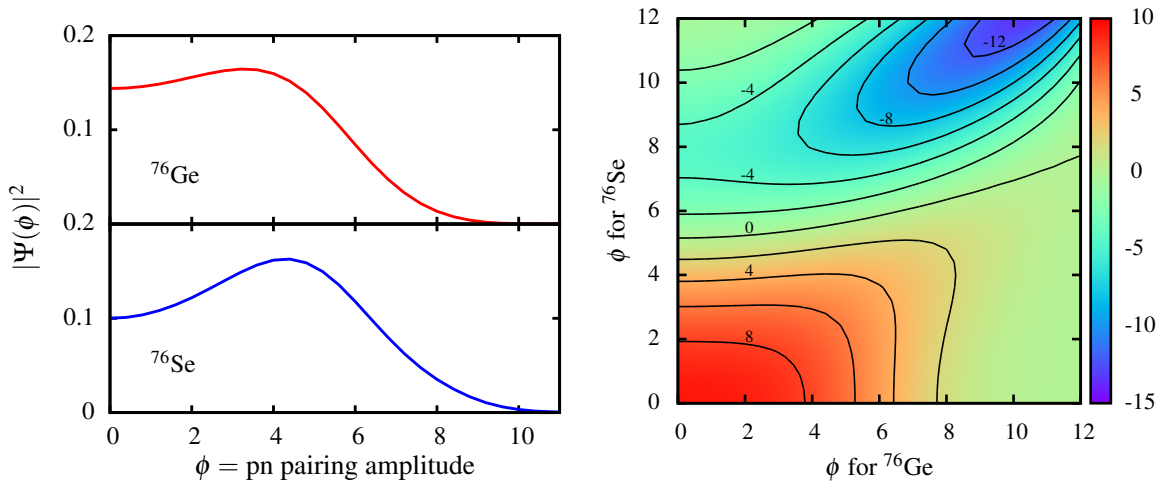


Figure 3: Left: Squares of collective wave functions, as a function of the proton-neutron pairing amplitude ϕ in ^{76}Ge (top) and ^{76}Se (bottom), the initial and final nuclei in the decay of ^{76}Ge , for the same Hamiltonian (2) as used for Fig. 2. Right: $0\nu\beta\beta$ matrix element as a function of the pairing amplitudes in the projected mean-field states making up the ground states of the initial and final nuclei. The matrix element has a maximum for no proton-neutron pairing and is reduced at the point at which the collective wave functions peak.

so by imposing constraints on both the quadrupole moment and the proton-neutron pairing amplitude, that is by minimizing

$$H' = H - \lambda_Z N_Z - \lambda_N N_N - \lambda_Q Q_{20} - \frac{\lambda_P}{2} (P_0 + P_0^\dagger), \quad (4)$$

where the Lagrange multipliers λ_Z and λ_N fix the expectation values of the proton and neutron number operators N_Z and N_N — this is part of the usual HFB minimization — and the other multipliers fix the quadrupole moment $\langle Q_{20} \rangle$ and the proton-neutron pairing amplitude $\phi \equiv \langle P_0 + P_0^\dagger \rangle$. Such a minimization requires generalizing the usual BCS-like wave functions to include proton-neutron, leading to quasiparticles that are part proton and part neutron as well part particle and part hole (which they are even in the usual treatment).

Ref. [17] carries out this calculation. With the quadrupole moment turned off, it produces “collective wave functions” of the proton-neutron pairing amplitude, the squares of which appear on the left side of Fig. 3. These represent the probability that the final diagonalized ground states in Ge and Se contain a given proton-neutron pairing amplitude $\phi = \langle P_0 + P_0^\dagger \rangle$. One can see that the wave functions are peaked around $\phi = 4$ or 5 . The right side of the figure shows the $0\nu\beta\beta$ matrix element as a function of the two pairing amplitudes. At the point representing the peak of the two wave functions, the matrix element is noticeably smaller than the point at which the

pairing amplitudes are zero. Finally, the part of Fig. 2 I haven't focused on shows the $0\nu\beta\beta$ matrix element as a function of the proton-neutron pairing strength. The GCM curve mirrors that produced by the QRPA until a point close to the mean-field phase transition, around and after which it behaves smoothly (as it should; there's no real phase transition beyond mean-field theory). The matrix element is indeed smaller than that of the ordinary GCM, which captures no proton-neutron correlations of this type and thus produces a result that is independent of g_{pn} .

The next step in the development of this approach is to move beyond the semi-realistic calculation discussed here and marry this enlarged GCM with sophisticated Skyrme or Gogny density functionals, which work in complete single-particle spaces, with all the nucleons active. The result will almost certainly be matrix elements that are closer to those of the shell model.

I turn finally to the renormalization of the axial-vector coupling g_A . It has been known for some time (see, e.g., Ref. [9]) that matrix elements for β and $2\nu\beta\beta$ decay are smaller in reality than in our calculations. If $0\nu\beta\beta$ matrix elements are as small compared to our calculations as $2\nu\beta\beta$ matrix elements, experiments are in trouble. Fortunately, the issue can now be investigated systematically. There can only be two sources of the quenching: many-body weak currents, which would alter the predictions of calculations with the one-body Gamow-Teller operator, and model space truncation, i.e. the omission of important configurations. Work is now beginning to examine both these sources. The effects of many-body currents have traditionally been thought to be small [18], but the construction of those currents in chiral effective field theory — currents that should go along with the interactions used by ab initio calculations — may lead to larger effects [19, 20]. Crucially, however, those effects should be smaller for $0\nu\beta\beta$ decay than for $2\nu\beta\beta$ decay. The issue should be cleared up by careful EFT parameter fits in the near future. The other source of quenching, model-space truncation, can be investigated in the ab initio shell-model calculations described earlier. Those implicitly include many configurations from outside the model space in the effective interactions and operators. We should soon be able to see whether $0\nu\beta\beta$ decay is quenched, and if so, by how much.

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